

# Laminar burning velocity of 2-methylfuran-air mixtures at elevated pressures and temperatures: Experimental and modeling studies

Xu, C., Zhong, A., Wang, H., Jiang, C., Sahu, A., Zhou, W. & Wang, C

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2     **Laminar Burning Velocity of 2-Methlfuran-air Mixtures at Elevated Pressures and**

3                     **Temperatures: Experimental and Modeling Studies**

4

5                     Cangsu Xu<sup>a</sup>, Anhao Zhong<sup>a</sup>, Hanyu Wang<sup>a</sup>, Changzhao Jiang<sup>b</sup>, Amrit Sahu<sup>c</sup>,

6                                     Wenhua Zhou<sup>a</sup>, Chongming Wang<sup>d\*</sup>

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9     <sup>a</sup> *College of Energy Engineering, Zhejiang University, Hangzhou, China, 310027*

10    <sup>b</sup> *Aeronautical and Automotive Engineering, Loughborough University, Leicestershire, United Kingdom, LE11 3TU*

11    <sup>c</sup> *Department of Mechanical Engineering, University of Birmingham, Birmingham, United Kingdom, B15 2TT*

12    <sup>d</sup> *School of Mechanical, Aerospace and Automotive Engineering, Coventry University, Coventry, United Kingdom, CV1 5FB*

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\* Corresponding author e-mail: [ac8174@coventry.ac.uk](mailto:ac8174@coventry.ac.uk)

**Abstract:** 2-Methylfuran (MF), a promising biofuel candidate catalytically produced from biomass-based fructose, has attracted the attention of fuel researchers. However, there is limited data available for the laminar burning velocity, especially at high initial pressure conditions. In this work, the laminar burning velocity of MF-air mixtures at elevated initial pressures ( $T_0 = 363$  K;  $p_0 = 0.1$ - $0.4$  MPa) was experimentally determined in a spherical outwardly expanding flame. Numerical simulation was also conducted in Chemkin using two detailed chemical kinetic mechanisms at elevated pressures (similar to the experiment condition:  $T_0 = 363$  K;  $p_0 = 0.1$ - $0.4$  MPa) and elevated temperatures ( $T_0 = 363$ - $563$  K;  $p_0 = 0.1$  MPa). Data from experimental and modelling studies were compared and discussed. The experimental results showed that at a given  $T_0$  and  $p_0$  the laminar burning velocity of MF-air mixtures reached peak values at equivalence ratios  $\phi = 1.1$ - $1.2$ , and it slowed down dramatically when the MF-air mixture was too rich or lean. Laminar burning velocity decreased with the increase in  $p_0$ . The laminar flame speed of MF-air mixture from two chemical kinetic mechanisms exhibited a similar trend with experimental data; however, both the two mechanisms led to overestimation at the most initial conditions. Compared to the Galway mechanism, the Tianjin mechanism better predicted the laminar burning velocity of MF-air mixtures, especially at initial pressures of  $0.1$  and  $0.2$  MPa. The current MF mechanism needs further improvement to better predict the combustion of MF at high-pressure conditions.

**Keywords:** 2-methylfuran; biofuel; laminar burning velocity; chemical kinetic mechanism

<b>MF</b>	2-Methylfuran	<b><math>\alpha</math></b>	Stretch rate
<b><math>p_0</math></b>	Initial pressure	<b><math>L_b</math></b>	Markstein length
<b><math>T_0</math></b>	Initial temperature	<b><math>u_L</math></b>	Laminar burning velocity
<b><math>A</math></b>	Area of flame front	<b><math>\rho_u</math></b>	Density of unburned gas
<b><math>t</math></b>	Time after ignition event	<b><math>\rho_b</math></b>	Density of burned gas
<b><math>R_0</math></b>	Radius of window	<b><math>\phi</math></b>	Equivalence ratio
<b><math>r_f</math></b>	Flame radius	<b><math>S_b</math></b>	Stretched flame propagation speed
<b><math>N</math></b>	Number of pixels inside the flame front	<b><math>S_u</math></b>	Unstretched flame propagation speed
<b><math>N_{all}</math></b>	Number of pixels of the entire window		

## 1. Introduction

Due to the pressures of greenhouse gas emission and limited fossil fuel resources, it is essential to find alternative fuels. Over the past decade, researchers have paid attention to biofuels, such as bioethanol [1, 2], biobutanol [3, 4] and biodiesel [5, 6]. Bioethanol is widely used as a gasoline blending stock because of its renewability, high-octane rating, low carbon footprint and regulation mandatory [7, 8]. However, bioethanol has its limitation, such as low calorific value and water solubility [9].

Román-Leshkov et al. [10] proposed a method of producing furan-based fuel, 2-methylfuran (MF), from biomass-based fructose via acid-catalyzed dehydration and hydrogenolysis processes. The properties of MF are listed in Table 1. Compared to bioethanol and gasoline, MF has several advantages [9]: (1) research octane number (RON) of MF is higher than that of gasoline; (2) the low heating value of MF is much higher than that of bioethanol; (3) unlike ethanol, MF is water-insoluble; (4) the enthalpy of vaporization of MF is lower than that of ethanol, indicating less cold start issues than ethanol.

**Table 1:** Properties of MF, bioethanol and gasoline [11, 12]

	Gasoline*	Bioethanol	MF
Molecular formula	C <sub>4</sub> -C <sub>12</sub>	C <sub>2</sub> H <sub>6</sub> O	C <sub>5</sub> H <sub>6</sub> O
Density @ 20°C (kg/m <sup>3</sup> )	744.6	790.9	913.2
Initial boiling point (°C)	33	78	64
Research Octane Number	96.8	108	103
Lower heating value (MJ/kg)	42.9	26.8	31.2
Oxygen content (wt.%)	0	34.78	19.51
Enthalpy of vaporization (kJ/kg)	351	919.6	389
Stoichiometric air-fuel ratio (gravimetric)	14.46	8.95	10.05

\* Typical main-grade EU gasoline that meets the EN228 regulation

MF has attracted the attention of engine researchers worldwide. Thewes et al. [13] experimentally investigated the influence of MF on spray, evaporation and engine performance in a direct-injection spark-ignition engine. They concluded that MF had quicker vaporisation compared to ethanol, and it had lower hydrocarbon emissions and better knock resistance compared to gasoline. Wang et al. [12] studied the combustion performance and emissions of MF in a direct-injection spark-ignition engine, and they compared the results with those of ethanol and gasoline. The results showed that MF had a better knock suppression ability and a higher indicated thermal efficiency than gasoline had. The particulate emissions from MF were less than gasoline

due to its high oxygen contents. However,  $\text{NO}_x$  emissions of MF were the highest among the four examined fuels because of its high combustion temperature.

Apart from pure MF, MF-gasoline blends were used as fuels in engines. Wei et al. [14] compared a MF-gasoline blend (M10), ethanol-gasoline (E10) and gasoline in a port-fuel-injection spark ignition engine. With less brake specific fuel consumption, the output torque and brake power of M10 were slightly higher than those of E10. Hydrocarbon and carbon monoxide emissions of M10 were lower than gasoline. Studies go beyond the application of SI engines. Xiao et al. [15] studied combustion performance and emissions of MF-diesel blend fuels in a diesel engine and they concluded that a low MF-diesel blend exhibited a longer ignition delay, a shorter combustion duration and lower soot emissions than pure diesel.

In addition to engine researches, fundamental combustion investigations of MF have been conducted. Somers et al. [16] established a detailed kinetic model of MF oxidation and validated it by experimental ignition delay times and laminar burning velocities. The model highlighted the reactions of the H atom with the fuel. Tran et al. [17] used electron-ionization molecular-beam mass spectrometry and gas chromatography techniques to detect the intermediate species of MF combustion under stoichiometric and fuel-rich premixed low-pressure flames conditions. They developed a detailed kinetic model consisting of 305 species and 1472 reactions. In addition, Cheng et al. [18] analysed the reaction pathway of MF and revised the former MF mechanism under fuel-lean, stoichiometric and fuel-rich conditions. Their mechanism was validated experimentally by detecting the mole fractions of major species in MF flames.

Laminar burning velocity is an important physiochemical parameter of a fuel-air mixture at given temperature and pressure conditions. The knowledge of laminar burning velocity is fundamental to the understanding of other more complicated flame behaviours such as flame extinction, flashback and turbulence combustion. Laminar burning velocity determined in experiments is also used to validate chemical kinetic mechanisms [19]. Laminar burning characteristics of MF and its blends with isooctane have been investigated at the atmospheric pressure, using an outwardly spherical flame method [20, 21]. The results revealed that the laminar burning velocity of MF was faster than that of isooctane.

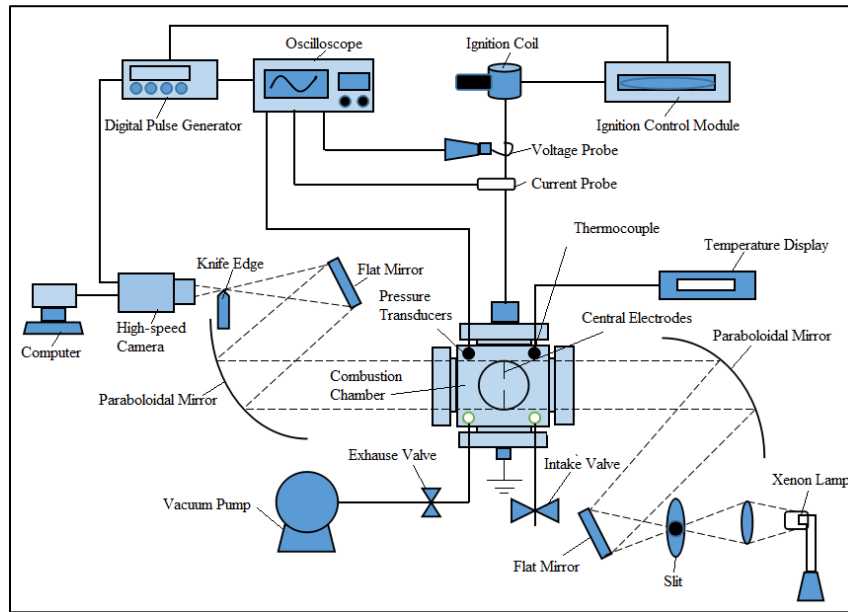
The laminar burning velocity of MF-air mixtures at high initial pressures is not available in the previous literature. In this work, the laminar burning velocity of MF-air mixtures at elevated initial

pressure ( $T_0 = 363$  K;  $p_0 = 0.1$ - $0.4$  MPa) was experimentally determined with a spherical outwardly expanding flame method. In addition to the experimental study, laminar burning velocity was also simulated by using two chemical kinetic mechanisms at elevated temperatures ( $T_0 = 363$ - $563$  K;  $p_0 = 0.1$ MPa) and elevated pressures ( $T_0 = 363$  K;  $p_0 = 0.1$ - $0.4$  MPa). Data from experimental and modelling studies were compared and discussed. In the next section, experimental and numerical methods will be introduced.

## 2. Experimental and Numerical Methods

### 2.1 Experimental Setup

Figure 1 presents the experimental setup. The system includes a constant-volume combustion chamber, a Schlieren photography system, an ignition system, an intake and exhaust system, and a data acquisition system.



**Figure 1:** Schematic of the experimental setup

The combustion vessel has a cubical shape, and it is equipped with a pair of quartz windows for the optical access. At each side, there were six cartridge heaters for temperature control. A K-type thermocouple and a pressure gauge were installed to measure the initial mixture temperature and pressure, respectively. Two opposing-electrodes with diameters of 0.4 mm were used for ignition along with an ignition coil and an ignition control module. Flame images were captured by a camera (speed=6000 fps; resolution=  $512 \times 512$ ). More details about these experimental apparatus and procedures are available in ref. [22, 23].

## 111 2.2 Data Processing

112 In this study, flame fronts of Schlieren images were determined via the Adobe Photoshop  
113 software. The radius ( $r_f$ ) of spherical flame is calculated via:

$$114 \quad r_f = \sqrt{\frac{N}{N_{\text{all}}}} R_w \quad (1)$$

115 where  $N$ ,  $N_{\text{all}}$  and  $R_w$  are the pixels inside the flame front, the pixels of the optical window, and the  
116 actual radius of the optical window, respectively.

117 The stretched flame propagation speed ( $S_b$ ) is calculated via:

$$118 \quad S_b = \frac{dr_f}{dt} \quad (2)$$

119 where  $t$  is the elapsed time after ignition.

120 In spherical expanding flames, the stretch rate ( $\alpha$ ) is defined as [24]:

$$121 \quad \alpha = \frac{2S_b}{r_f} \quad (3)$$

122 According to [25], during the quasi-steady period stretched propagation speed and stretch rate  
123 have linear relationship:

$$124 \quad S_b = S_u - L_b \alpha \quad (4)$$

125 where  $S_u$  is the unstretched flame propagation speed;  $L_b$  is the Markstein length relative to the  
126 burned gas.

127 With the assumption of a quasi-steady and quasi-planar flame, laminar burning velocity ( $u_L$ ) is  
128 calculated based on the law of mass conservation across the flame front [25]:

$$129 \quad u_L = \frac{\rho_b}{\rho_u} S_u \quad (5)$$

130 where  $\rho_b$  and  $\rho_u$  are the densities of the burned and unburned gas, respectively.

131

## 132 2.3 Experimental Uncertainty Analysis

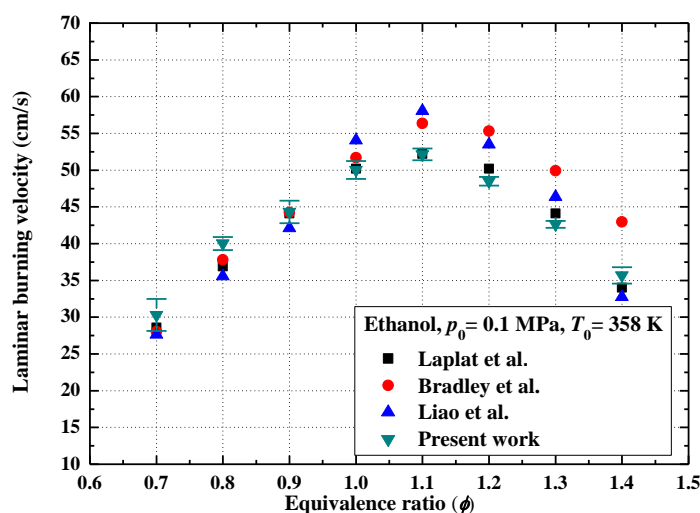
133 The primary experiment errors are caused by the uncertainty of initial temperature ( $\Delta U_T$ ), initial  
134 pressure ( $\Delta U_p$ ), the number of pixels inside the flame front ( $\Delta U_A$ ), the vessel effective volume ( $\Delta U_V$ )  
135 and the fuel metering ( $\Delta U_F$ ). The accuracy of K-type thermocouples used in this work is  $\pm 0.75\%$ ,  
136 and the perturbation of initial temperature can lead to an uncertainty of  $\sim 0.8\%$  in the determination



137 of laminar burning velocity at 0.1 MPa, while at 0.4 MPa the uncertainty can reach ~1.5% [26]. The  
 138 resolution of the pressure transducer is 0.0001 MPa, and the uncertainty caused by initial pressure is  
 139 less than 0.1%. In addition, the uncertainty of the pixels inside the flame front is estimated to be  
 140 ~1%. The uncertainty of the vessel effective volume is ~0.2%. The fuel metering is via a glass  
 141 syringe with a capacity of 250  $\mu\text{L}$  and with a resolution of 5  $\mu\text{L}$ , and the uncertainty is dependent on  
 142 the quantity of fuel required for each test condition. In summary, the global laminar burning  
 143 velocity uncertainty ( $\sqrt{\Delta U_T^2 + \Delta U_p^2 + \Delta U_A^2 + \Delta U_V^2 + \Delta U_F^2}$ ) is within 2% for all the laminar burning  
 144 velocities tested in this work, and the global equivalent ratio is within 2.5%.

## 145 2.4 System Validation

146 Laminar burning velocity of ethanol-air mixtures were measured at  $T_0 = 358 \text{ K}$  and  $p_0 = 0.1 \text{ MPa}$ .  
 147 Figure 2 shows the current results and those from Liao et al. [27], Bradley et al. [28] and Laplat et  
 148 al. [29]. The measurement results in this work are close to those from others; in particular, the  
 149 average deviation between present results and data reported in Ref. [29] was ~0.01 m/s. This can  
 150 prove the experimental setup and method in this work are reliable.



151  
 152 **Figure 2:** Laminar burning velocities of ethanol-air mixtures measured by the authors' system  
 153 and presented in the literature ( $T_0 = 358 \text{ K}$  and  $p_0 = 0.1 \text{ MPa}$ )  
 154

## 155 3. Modelling of Laminar Burning Velocity

156 Two chemical kinetic mechanisms developed by researchers from Tianjin University (Tianjin  
 157 Mechanism) [18] and NUI Galway (Galway Mechanism) [16,30-31] were used to simulate the  
 158 laminar burning velocity of MF-air mixtures in Chemkin.

159 The Galway mechanism is a detailed chemical kinetic mechanism, consisting of 391 species  
160 and 2059 reactions [16,30-31]. This mechanism references several sub-mechanisms from the  
161 literature: furan mechanisms [32, 33], aromatic mechanisms [34], H<sub>2</sub> and CO mechanisms [35, 36],  
162 light hydrocarbon mechanisms (C<sub>1</sub>–C<sub>3</sub>) [37, 38], saturated C<sub>4</sub> mechanism [39] and unsaturated C<sub>4</sub>  
163 mechanism [40].

164 The Tianjin mechanism is a detailed chemical kinetic mechanism, consisting of 586 species and  
165 2997 reactions. It is developed based on the Galway Mechanism [30,31]. The Tianjin mechanism  
166 updated and emerged some important reactions from Galway Mechanism, such as the reactions  
167 related to C<sub>3</sub>H<sub>3</sub>, benzene, benzyl and fulvene. More fractions of some key species such as MF22J  
168 and P134TE1O are quantitatively measured to analyse the pathway of MF.

169

## 170 **4. Results and Discussion**

171 This section consists of two parts. In the first part, experimental results of the laminar burning  
172 velocity for MF-air mixture at elevated initial pressures ( $T_0 = 363$  K,  $p_0 = 0.1$ - $0.4$  MPa) are  
173 presented. Before those experimental results are presented, four criteria of flame front radius  
174 selection for the determination of laminar burning velocity are discussed. In the second part, results  
175 from modelling study using two MF chemical kinetics mechanisms are provided. The modelling  
176 study covers the all test condition as the experiments ( $T_0 = 363$  K,  $p_0 = 0.1$ - $0.4$  MPa), and the results  
177 from modelling and experiments are compared. In addition, the simulation extends to elevated  
178 initial temperatures ( $T_0 = 363$ - $563$  K,  $p_0 = 0.1$ MPa).

179

### 180 **4.1 Experimental Study**

#### 181 **4.1.1 Flame radius selection**

182 There are four criteria for the selection of flame front radius for the determination of laminar  
183 burning velocity.

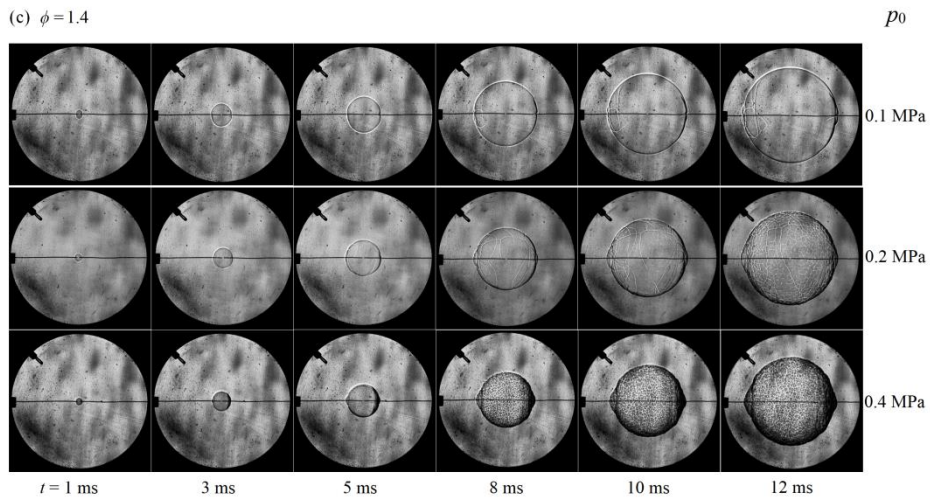
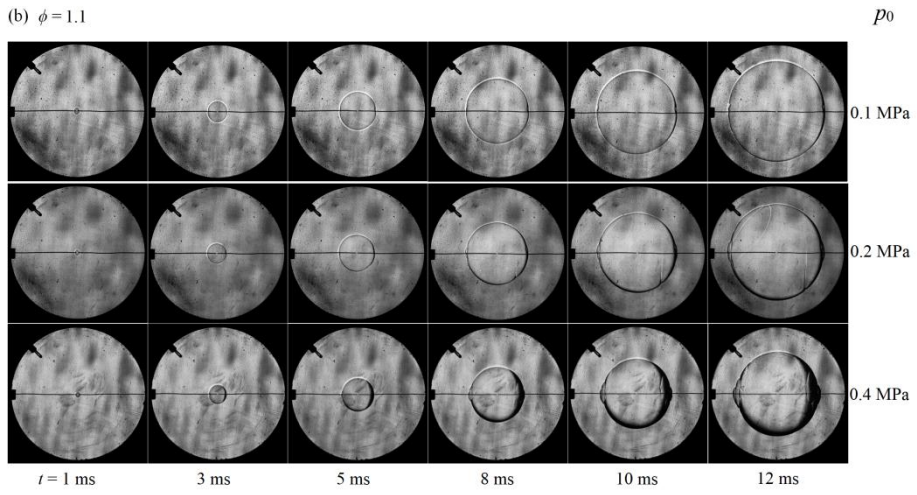
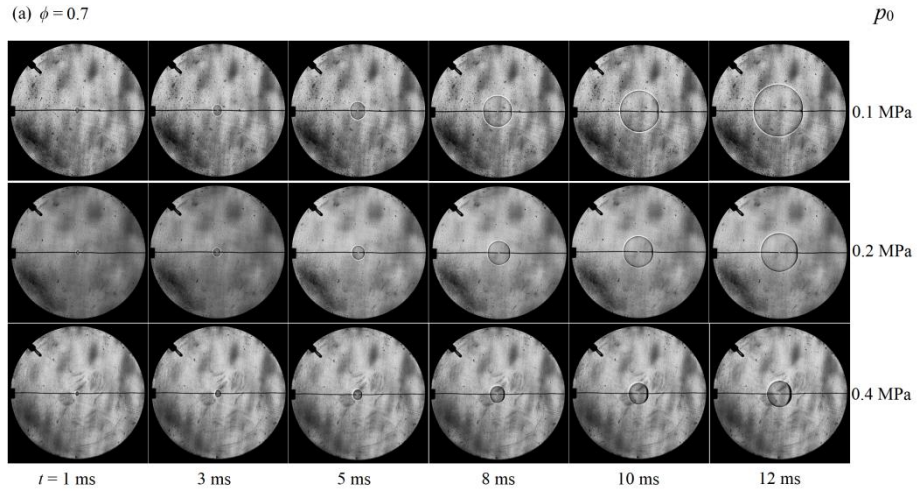
184 **Spark- and wall-affected periods:** The development of a spherical outwardly expanding flame  
185 in a constant-volume vessel consists of three distinctive periods: an initial period affected by the  
186 ignition energy, followed by a quasi-steady period and a final period influenced by the chamber  
187 confinement [26]. Laminar flame speed, the value of stretched flame speed extrapolated at zero  
188 stretch rate, can be determined from a spherical outwardly expanding flame in a constant-volume

189 vessel; however, not all the aforementioned stages of flame propagation is suitable for determining  
190 the laminar burning velocity. The spark-affected and wall confinement-affected stages need to be  
191 identified and be excluded. In this work, flame radii between 8 and 20 mm were used in the  
192 determination of laminar burning velocity, which can effectively avoid the spark- and wall-affected  
193 periods. Similar flame radii ranges were selected by many research groups [41-43]. It should be  
194 noted that the exact range is dependent on the geometry of the vessel and ignition system.

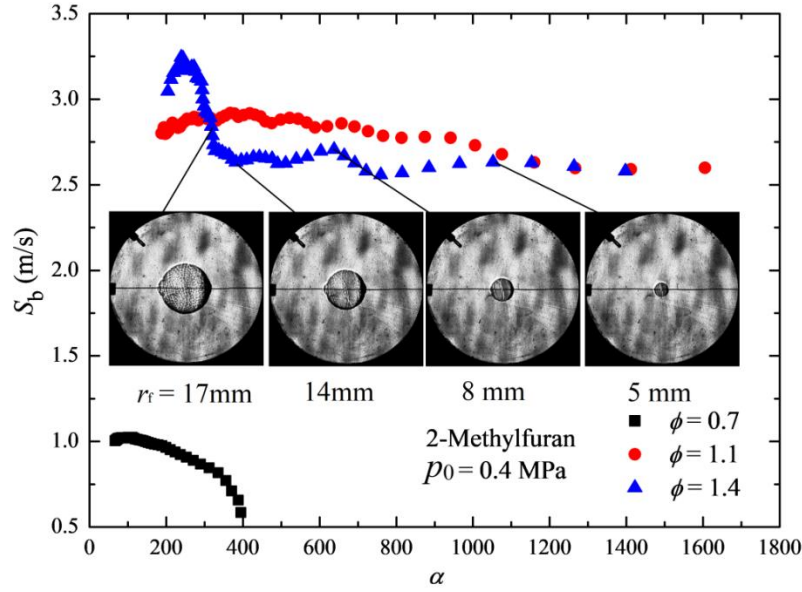
195 **Flame instability and self-acceleration:** There is a phenomenon that makes the laminar  
196 burning velocity determination difficult at high initial pressure condition in a vessel. At a certain  
197 flame propagation stage, flame front becomes unstable, and wrinkle structures appear on the flame  
198 surface. The flame front will be accelerated after a critical flame radius, which is the onset point for  
199 the unstable flame. If the critical flame radius is too small, the flame radius window suitable for  
200 laminar burning velocity calculation will be too small, leading to inaccurate laminar burning  
201 velocity. The flame instability can be observed directly from Schlieren images or from the flame  
202 propagating speed.

203 Figure 3 presents the Schlieren flame images of MF-air mixtures at different  $p_0$  and  $\phi$ .  $p_0$  and  $\phi$   
204 had significant impacts on the development of flame morphology. At  $\phi = 0.7$ , the flame surface was  
205 smooth at all tested  $p_0$ , indicating that the flame was stable. At  $\phi = 1.1$ , the flame surface was  
206 smooth at  $p_0 = 0.1$  MPa; however, it developed some cracks/wrinkles, and there were obvious  
207 protuberances on the area that in contact with ignition wires at  $p_0 = 0.2$ - $0.4$  MPa, indicating that the  
208 flame was unstable. The flame instability was more obvious at  $\phi = 1.4$ , where the clear  
209 cellularization was observed at  $p_0 = 0.2$ - $0.4$  MPa. In addition, flame surface cellularization appeared  
210 earlier at  $p_0 = 0.4$  MPa than at  $p_0 = 0.2$  MPa. Therefore, the flame instability increased with the  
211 increase of  $p_0$  and  $\phi$ .

212



**Figure 3:** Schlieren images of MF-air mixture flame at  $T_0 = 363$  K,  $p_0 = 0.1$ - $0.4$  MPa: (a)  $\phi = 0.7$ ; (b)  $\phi = 1.1$ ; and (c)  $\phi = 1.4$

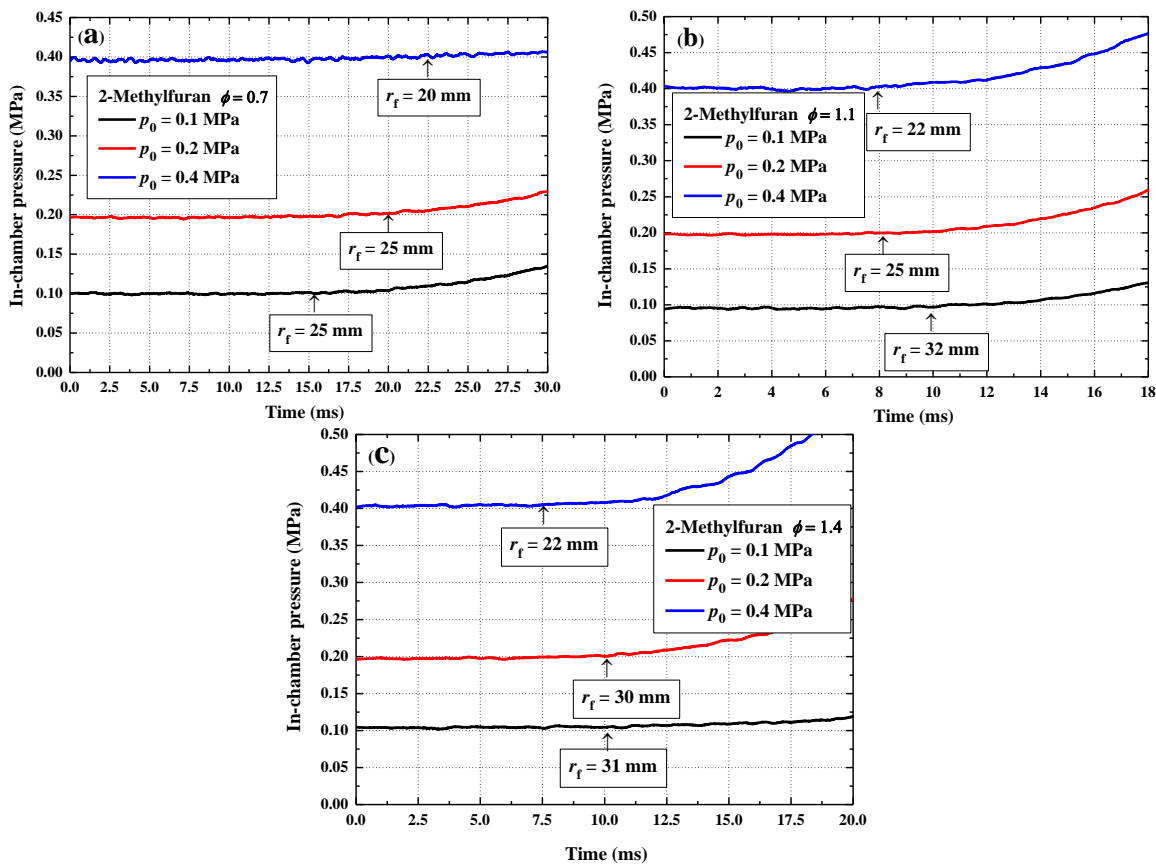


**Figure 4:** Stretched flame propagation speed versus stretch rate of MF-air mixtures at  $T_0 = 363$  K,  $p_0 = 0.4$  MPa, and  $\phi = 0.7, 1.1$  and  $1.4$

Flame surface cellularization may lead to flame self-acceleration. Figure 4 plots stretched flame propagation speed ( $S_b$ ) versus stretch rate ( $\alpha$ ) ( $T_0 = 363$  K,  $p_0 = 0.4$  MPa,  $\phi = 0.7, 1.1$  and  $1.4$ ). Some key flame images and flame radius are provided in Figure 4. It can be seen that at  $\phi = 1.4$ , initially,  $S_b$  varied little with  $\alpha$ , but  $S_b$  suddenly increased dramatically at the flame radius of 14 mm. In this study, the determination of laminar burning velocity excluded the flame radius where the flame was unstable or flame self-acceleration was observed.

**Pressure:** Pressure inside the chamber will increase after the flame develops to a certain size. However, there is an assumption for the use of Equation (2)-(5) to determine the laminar burning velocity: in-vessel pressure must be constant [44]. Figure 5 shows the in-chamber pressure versus time after ignition event of MF-air mixtures at  $T_0 = 363$  K,  $p_0 = 0.1$ - $0.4$  MPa and  $\phi = 0.7, 1.1$  and  $1.4$ . Flame radius where the pressure started to increase is marked in Figure 5. It is obvious that before the flame radius of 20 mm, no clear in-chamber pressure rise was observed.

Only a small window of flame propagation would be selected for the determination of laminar burning velocity, excluding the effects of ignition energy, chamber wall confinement, flame instability and self-acceleration, and pressure rise. In this work, flame radii between 8 and 20 mm were used for safe determination of laminar burning velocity. For rich MF-air mixtures at 0.4 MPa, the maximum flame radius was decreased to 14 mm due to the cellular structure and self-acceleration.



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#### 244 4.1.2 Laminar burning velocity from experimental study

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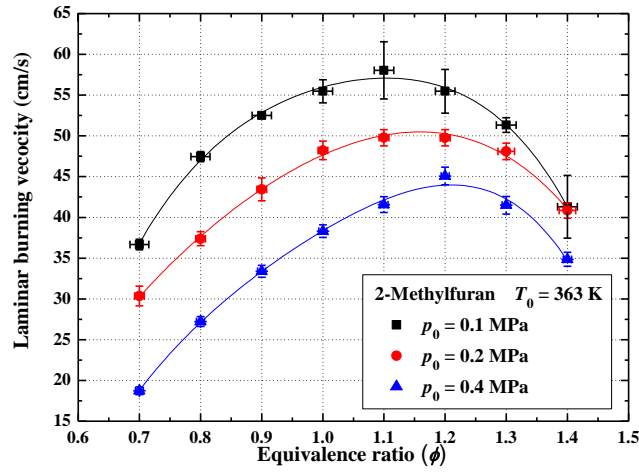
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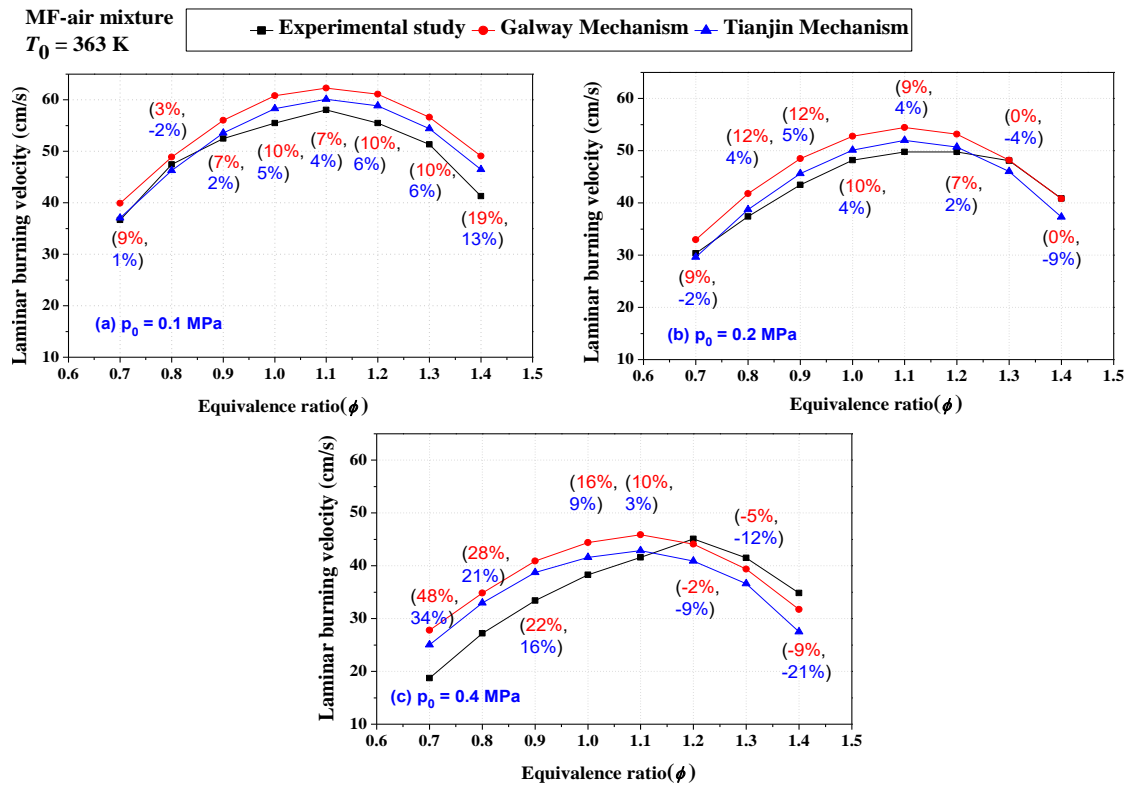
**Figure 5:** In-chamber pressure versus time after ignition event of MF-air mixtures at  $T_0 = 363$  K and  $p_0 = 0.1$ - $0.4$  MPa: (a)  $\phi = 0.7$ ; (b)  $\phi = 1.1$ ; and (c)  $\phi = 1.4$

Figure 6 shows the laminar burning velocity versus  $\phi$  at  $T_0 = 363$  K and  $p_0 = 0.1$ - $0.4$  MPa. As  $p_0$  increased, laminar burning velocity decreased, due to the increased rates of the three-body recombination reactions [45]. This trend is consistent with the results of other fuels, such as ethanol [28] and DMF [45]. Within the range of  $\phi = 0.7$ - $1.1$ , the laminar burning velocity at  $p_0 = 0.1$  MPa was averagely 16.6% and 37.5% faster than that at  $p_0 = 0.2$  MPa and  $p_0 = 0.4$  MPa, respectively. The peak value of laminar burning velocity was occurred at  $\phi = 1.1$  at  $p_0 = 0.1$  and  $0.2$  MPa, and at  $\phi = 1.2$  at  $p_0 = 0.4$  MPa.



**Figure 6:** Laminar burning velocity of MF-air mixtures at  $T_0 = 363$  K and  $p_0 = 0.1$ - $0.4$  MPa

## 4.2 Modeling Simulation

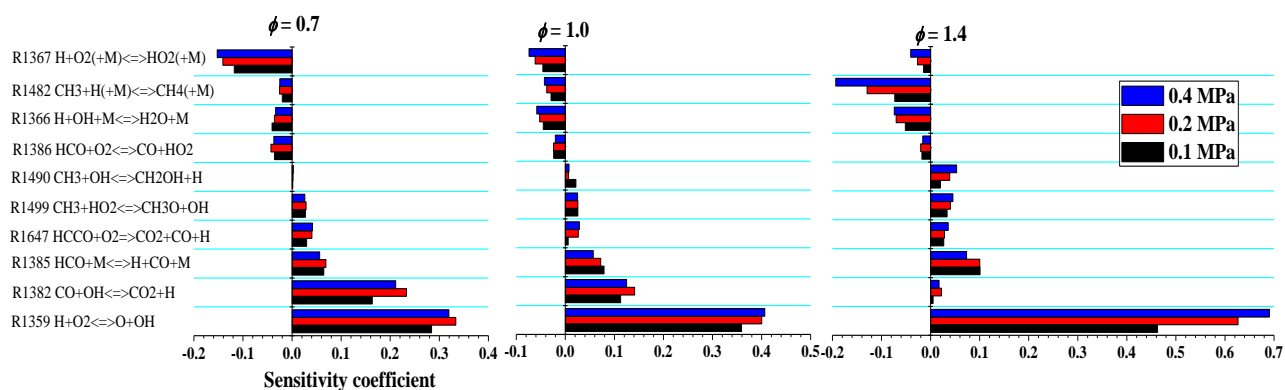


**Figure 7:** Comparison of experimental and simulated laminar burning velocity of MF-air mixtures at  $T_0 = 363$  K and  $p_0 = 0.1$ - $0.4$  MPa

Figure 7 shows the laminar burning velocities of MF-air mixtures at  $T_0 = 363$  K and  $p_0 = 0.1$ - $0.4$  MPa, simulated in two chemical kinetic mechanisms developed by researchers from Tianjin University (Tianjin Mechanism) and NUI Galway (Galway Mechanism), and the simulation results



are compared with experimental data in this research. Results from both mechanisms show that laminar burning velocity reached the maximum value at given initial  $T_0$  and  $p_0$  at approximately  $\phi = 1.1$ , and the laminar burning velocity profile was symmetric with respect to  $\phi = 1.1$ . This finding is similar to the experimental results shown in Figure 6. There are two numbers in the bracket near each data point in Figure 7: the top number means the percentage difference between results from experiments and Galway mechanism; the bottom number means the percentage difference between results from experiments and Tianjin mechanism. It can be seen that both Galway and Tianjin mechanisms overestimated laminar burning velocities of MF-air mixtures at most conditions, apart from for rich mixtures ( $p_0 = 0.2$  and  $0.4$  MPa) where both mechanisms gave underestimated laminar burning velocities. Comparing two mechanisms, the results from Tianjin mechanism was closer to the experimental results, especially at the initial pressure of  $0.1$  and  $0.2$  MPa (the percentage difference was mostly less than  $6\%$ ). Because the authors of Tianjin mechanism measured the mole fractions of several important intermediate products (MF22J, P134TE1O, etc.), and analysed the reaction pathways of MF combining the Galway mechanism and their experimental data. However, the discrepancy became larger for lean and rich conditions (the percentage difference was more than  $20\%$ ) at the initial pressure of  $0.4$  MPa. The mechanism needs further modification to be used for high-pressure simulation.

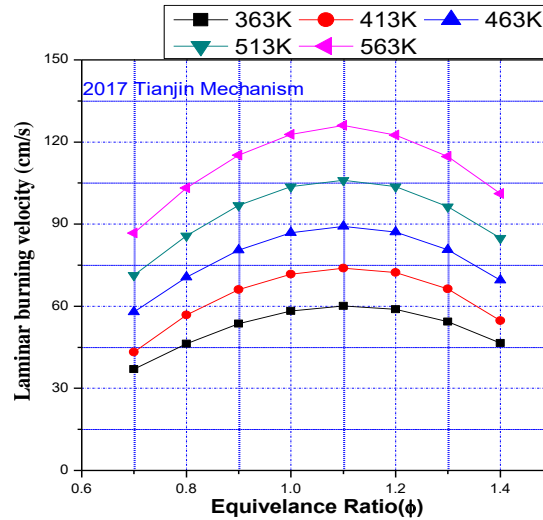


**Figure 8:** Sensitivity analyses of MF-air flames using Tianjin mechanism at three different equivalence ratios ( $0.7$ ,  $1.0$  and  $1.4$ ) and three initial pressures ( $0.1$ ,  $0.2$  and  $0.4$  MPa)

Figure 8 shows the sensitivity analyses of MF-air flame at different equivalence ratios and different initial pressures. The sensitivity analyses were conducted for the Tianjin mechanism. The influence of rate constant of each reaction on the flame speed was reflected by the sensitivity coefficient. The most important reaction was R1359, which increased the number of active radicals



287 in flame; and its sensitivity coefficient was increased with the increase of equivalence ratio and  
 288 initial pressure, except for the situation from 0.2 to 0.4 MPa at  $\phi = 0.7$ . For lean and stoichiometric  
 289 conditions, the oxidation of CO to CO<sub>2</sub> by OH (R1382) had a significant positive effect on flame  
 290 speed, and the sensitivity coefficient was decreased with the increase of equivalence ratio. The  
 291 decomposition of HCO (R1385) increased the flame speed to some extent. In addition, the flame  
 292 speed was slightly promoted by R1499 and R1647 for all the initial conditions; and for rich  
 293 conditions, the flame speed could also be increased by R1490. There exists some reactions with  
 294 negative sensitivity coefficient which inhibit the flame speed. Reactions had large inhibiting effect  
 295 were three-body reactions, such as the combinations of H and O<sub>2</sub> (R1367), CH<sub>3</sub> and H (R1482), and  
 296 H and OH (R1366), etc. The sensitivity coefficients of them were decreased with the increase of  
 297 initial pressure. Since the three-body reactions are the key reactions in reproducing the experiments  
 298 at higher initial pressure. Therefore, the three-body reactions should be further modified to better  
 299 reproduce the experiment at higher pressures.



300  
 301 **Figure 9:** Simulated laminar burning velocity of MF-air mixtures at  $T_0 = 363\text{-}563$  K and  $p_0 =$   
 302 0.1MPa (Tianjin Mechanism)

303 The simulation is extended to conditions beyond the experimental conditions. Figure 9 shows  
 304 the laminar burning velocity of MF-air mixtures at  $T_0 = 363\text{-}563$  K and  $p_0 = 0.1\text{MPa}$ , simulated by  
 305 the Tianjin Mechanism. Again, the laminar burning velocity trend with respect to  $\phi$  is highly similar  
 306 to the results shown in Figure 7. At a given equivalence ratio, the laminar burning velocity increases  
 307 with  $T_0$ , and the increase rate is positive. This was caused by the enhanced chemical reaction rate at  
 308 a higher temperature.

309

## 310 5. Conclusions

311 In this work, an experimental study of the laminar burning velocity of MF-air mixtures at  
312 elevated initial pressure ( $T_0 = 363$  K;  $p_0 = 0.1$ - $0.4$  MPa) was conducted in the spherical outwardly  
313 expanding flame. Laminar burning velocity was also simulated in Chemkin using two chemical  
314 kinetic mechanisms at elevated initial temperatures ( $T_0 = 363$ - $563$  K;  $p_0 = 0.1$ MPa) and elevated  
315 initial pressures ( $T_0 = 363$  K;  $p_0 = 0.1$ - $0.4$  MPa). Experiments show that the laminar burning velocity  
316 of MF-air mixtures was firstly increased and then decreased as the  $\phi$  increased from 0.7 to 1.4. At  
317 given  $p_0$  and  $T_0$ , the maximum values of laminar burning velocities were observed at  $\phi = 1.1$ - $1.2$ .  $p_0$   
318 had a negative influence on the laminar burning velocity. Simulation results showed a similar trend  
319 with experimental results; however, both the Tianjin and Galway mechanisms overestimated the  
320 laminar burning velocity of MF-air mixtures at most initial conditions, apart from for rich mixtures  
321 ( $p_0 = 0.2$  and  $0.4$  MPa) where both mechanisms gave underestimated laminar burning velocities.  
322 Compared to the Galway mechanism, the Tianjin mechanism consistently produced a more accurate  
323 prediction of the laminar burning velocity of MF-air mixtures. At the initial pressures of 0.1 and 0.2  
324 MPa, the percentage difference was almost less than 6%; however, at higher initial pressure ( $p_0 =$   
325  $0.4$  MPa), the discrepancy between experimental and simulation results became larger at lean and  
326 rich conditions (discrepancy  $> 20\%$ ). This shows that the current MF mechanism requires some  
327 revision for a better prediction of laminar flame speed at high initial pressure.

328

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